

Pairwise Entanglement and Geometric Phase in High Dimensional Free-Fermion Lattice Systems

H. T. Cui and Y. F. Zhang

Department of Physics, Anyang Normal University, Anyang, 455000, China, e-mail: cuiht@aynu.edu.cn

Received: February 17, 2009/ Revised version: February 17, 2009

Abstract. The pairwise entanglement, measured by concurrence and geometric phase in high dimensional free-fermion lattice systems have been studied in this paper. When the system stays at the ground state, their derivatives with the external parameter show the singularity closed to the phase transition points, and can be used to detect the phase transition in this model. Furthermore our studies show for the free-fermion model that both concurrence and geometric phase show the intimate connection with the correlation functions. The possible connection between concurrence and geometric phase has been also discussed.

PACS. 03.65.Vf Phases: geometric; dynamic or topological; 03.65.Ud Entanglement and quantum nonlocality; – 05.70.Fh Phase transitions: general studies

1 introduction

The understanding of quantum many-body effects based on the fundamentals of quantum mechanics, has been raising greatly because of the rapid development in quantum information theory [1]. Encouraged by the suggestion of Preskill [2], the connection between the quantum entanglement and quantum phase transition has been demonstrated first in 1D spin-1/2 XY mode [3], and then was extended to more other spin-chain systems and fermion systems (see Ref [1] for a review). Furthermore the decoherence of a simple quantum systems coupled with the quantum critical environment has been shown the significant features closed to the critical points [4, 5]. Regarding these findings, the fidelity between the states across the transition point has also been introduced to mark the happening of the phase transitions [6]. These intricate connections between quantum entanglement and phase transition in many-body systems have sponsored great effort devoted to the understanding of many-body effects from quantum information point [1]. In general quantum entanglement as a special correlation, is believed to play an essential role for the many-body effects since it is well accepted that the non-trivial correlation is at the root of many-body effects. Although the ambiguity exists [7], quantum entanglement provides us a brand-new perspective into quantum many-body effects. However the exact physical meaning of quantum entanglement in many body systems remains unclear [8]. Although the entanglement witnesses has been constructed in some many-body systems [9], a general and physical understanding of quantum entanglement in many-body systems is still absent.

On the other hand, the geometric phase, which was first studied systemically by Berry [10] and had been re-

searched extensively in the past 20 years [11], recently has also been shown the intimate connection to quantum phase transitions [12, 13, 14, 15, 16, 17, 18](or see a recent review Ref. [19]). This general relation roots at the topological property of the geometric phase, which depicts the curvature of the Hilbert space, and especially has direct relation to the property of the degeneracy in quantum systems. The degeneracy in the many-body systems is critical in our understanding of the quantum phase transition [20]. Thus the geometric phase is another powerful tool for detecting the quantum phase transitions. Moreover recently geometric phase has been utilized to distinguish different topological phases in quantum Hall systems [21], in which the traditional phase transition theory based on the symmetry-broken theory is not in function [22].

Hence it is very interesting to discuss the possible connection between entanglement and geometric phase, since both issues show the similar sensitivity to the happening of quantum phase transition. Recently the connection between the entanglement entropy and geometric phase has first been discussed with a special model in strongly correlated systems; the geometric phase induced by the twist operator imposed on the filled Fermi sphere, was shown to present a lower bound for the entanglement entropy [23]. This interesting result implies the important relation between quantum entanglement and geometric phase, and provides an possible understanding of entanglement from the topological structure of the systems. In another way the two-particle entanglement was also important [3]. Especially in spin-chain systems two-particle entanglement is more popular and general because of the interaction between spins, and furthermore the quantum information transferring based on spin systems are generally dependent on the entanglement between two particles [24]. So

it is a tempting issue to extend this discussion to the universal two-particle entanglement situation.

For this purpose the pairwise entanglement and geometric phase are studied systemically in this paper. Our discussion focuses on nearest-neighbor entanglement in the ground state in free-Fermion lattice systems because of the availability of the exact results. By our own knowledge, this paper first presents the exact results of entanglement and geometric phase in higher dimensional systems. In Sec.2 the model will be provided, and the entanglement measured by Wootter's concurrence is calculated by introducing pseudospin operators. Furthermore the geometric phase is obtained by imposing a globe rotation, and its relation with concurrence are also discussed generally. In Sec.3, we discussed respectively the concurrence and geometric phase in 2D and 3D cases. Finally, the conclusion is presented in Sec.4.

2 Model

The Hamiltonian for spinless fermions in lattice systems reads

$$H = \sum_{ij}^L c_i^\dagger A_{ij} c_j + \frac{1}{2} (c_i^\dagger B_{ij} c_j^\dagger + \text{h.c.}), \quad (1)$$

in which $c_i^{(\dagger)}$ is fermion annihilation(creation) operator and L is the total number of lattice sites. The hermiticity of H imposes that matrix A is Hermit and B is an anti-symmetry matrix. The configuration of lattice does not matter for Eq. (1) since our discussion focuses on the general case and available exact results. This model obviously is solvable exactly and can be transformed into the free Bogoliubov fermionic model. So it is also called free-fermion model. By Jordan-Wigner transformation [27] one can convert the spin-chain systems into spinless fermions systems, in which the physical properties can be readily determined. Therefore an alternative approach is necessary by which one can treat solvable fermion systems of arbitrary size. The model Eq. (1) serves this purpose.

Without the loss of generality we assume A and B to be real [25]. An important property of Eq. (1) is

$$[H, \prod_i^L (1 - 2c_i^\dagger c_i)] = 0. \quad (2)$$

This symmetry would greatly simplify the consequent calculation of the reduced density matrix for two fermions. One can diagonalize Eq. (1) by introducing linear transformation with real $g_{\mathbf{ki}}$ and $h_{\mathbf{ki}}$ [25]

$$\eta_{\mathbf{k}} = \frac{1}{\sqrt{L}} \sum_i^L g_{\mathbf{ki}} c_i + h_{\mathbf{ki}} c_i^\dagger, \quad (3)$$

in which the normalization factor $1/\sqrt{L}$ have been included to ensure the convergency under the thermodynamic limit. After some algebra, the Hamiltonian Eq. (1) becomes

$$H = \sum_{\mathbf{k}} \Lambda_{\mathbf{k}} \eta_{\mathbf{k}}^\dagger \eta_{\mathbf{k}} + \text{const.} \quad (4)$$

in which $\Lambda_{\mathbf{k}}^2$ is the common eigenvalue of the matrices $(A - B)(A + B)$ and $(A + B)(A - B)$ with the corresponding eigenvectors $\phi_{\mathbf{ki}} = g_{\mathbf{ki}} + h_{\mathbf{ki}}$ and $\psi_{\mathbf{ki}} = g_{\mathbf{ki}} - h_{\mathbf{ki}}$ respectively (see Ref. [25] for details). The ground state is defined as $|g\rangle$, which satisfies the relation

$$\eta_{\mathbf{k}} |g\rangle = 0 \quad (5)$$

With respect to fermi operator $\eta_{\mathbf{k}}$, one has relations

$$\begin{aligned} \frac{1}{L} \sum_i g_{\mathbf{ki}} g_{\mathbf{k'i}} + h_{\mathbf{ki}} h_{\mathbf{k'i}} &= \delta_{\mathbf{k'k}}^{(3)} \\ \frac{1}{L} \sum_i g_{\mathbf{ki}} h_{\mathbf{k'i}} + h_{\mathbf{ki}} g_{\mathbf{k'i}} &= 0 \end{aligned} \quad (6)$$

Furthermore the requirement that $\{\phi_{\mathbf{k}}, \forall \mathbf{k}\}$ and $\{\psi_{\mathbf{k}}, \forall \mathbf{k}\}$ be normalized and complete, reinforce the relations [25]

$$\begin{aligned} \frac{1}{L} \sum_{\mathbf{k}} g_{\mathbf{ki}} g_{\mathbf{kj}} + h_{\mathbf{ki}} h_{\mathbf{kj}} &= \delta_{ij} \\ \frac{1}{L} \sum_{\mathbf{k}} g_{\mathbf{ki}} h_{\mathbf{kj}} + h_{\mathbf{ki}} g_{\mathbf{kj}} &= 0 \end{aligned} \quad (7)$$

With the help of these formula above, one obtains

$$c_i = \frac{1}{\sqrt{L}} \sum_{\mathbf{k}} g_{\mathbf{ki}} \eta_{\mathbf{k}} + h_{\mathbf{ki}} \eta_{\mathbf{k}}^\dagger, \quad (8)$$

which would benefit our calculation for the correlation functions.

2.1 Concurrence

The concurrence, first introduced by Wootters [26] for the measure of two-qubit entanglement, is defined as

$$c = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}, \quad (9)$$

in which $\lambda_i (i = 1, 2, 3, 4)$ are the square roots of eigenvalues of matrix $R = \rho(\sigma^y \otimes \sigma^y) \rho(\sigma^y \otimes \sigma^y)$ with decreasing order. Then the critical step is to determine the two-body reduced density operator ρ . The reduced density operator ρ_{ij} for two spin-half particles labeled \mathbf{i}, \mathbf{j} can be written generally as,

$$\rho_{ij} = \text{tr}_{ij} \rho = \frac{1}{4} \sum_{\alpha, \beta=0}^3 p_{\alpha, \beta} \sigma_i^\alpha \otimes \sigma_j^\beta, \quad (10)$$

in which ρ is the density matrix for the whole system and σ^0 is the 2×2 unity matrix and $\sigma^\alpha (\alpha = 1, 2, 3)$ are the Pauli operators $\sigma^x, \sigma^y, \sigma^z$, which also the generators of $SU(2)$ group. $p_{\alpha\beta} = \text{tr}[\sigma_i^\alpha \sigma_j^\beta \rho_{ij}] = \langle \sigma_j^\alpha \sigma_i^\beta \rangle$ is the correlation function. With the symmetry Eq. (2), one can verify that only $p_{00}, p_{03}, p_{30}, p_{11}, p_{22}, p_{33}, p_{12}, p_{21}$ are not vanishing. After some efforts, one obtain

$$c = \max\{0, c_I, c_{II}\}, \quad (11)$$

in which

$$c_I = \frac{1}{2} [\sqrt{(p_{11} + p_{22})^2 + (p_{12} - p_{21})^2} - \sqrt{(1 + p_{33})^2 - (p_{30} + p_{03})^2}]$$

$$c_{II} = \frac{1}{2} [|p_{11} - p_{22}| - \sqrt{(1 - p_{33})^2 - (p_{30} - p_{03})^2}]. \quad (12)$$

In order to obtain the reduced density operator for two fermions, it is crucial to construct $SU(2)$ algebra for the fermions in lattice systems. In 1D case, the Jordan-Wigner (JW) transformation is available [27, 12, 13, 25]. For higher dimension cases the JW-like transformation has been constructed by different methods [28]. However the transformation is very complex and the calculation is difficult. Hence instead of a general calculation, we focus on the nearest neighbor two lattices in this paper. In this situation, the $SU(2)$ algebra can be readily constructed

$$\begin{aligned} \sigma_i^+ &= (\sigma_i^x + i\sigma_i^y)/2 = c_i^\dagger \\ \sigma_i^- &= (\sigma_i^x - i\sigma_i^y)/2 = c_i \\ \sigma_i^z &= 2c_i^\dagger c_i - 1 \\ \sigma_{i+1}^+ &= (\sigma_{i+1}^x + i\sigma_{i+1}^y)/2 = (2c_i^\dagger c_i - 1)c_{i+1}^\dagger \\ \sigma_{i+1}^- &= (\sigma_{i+1}^x - i\sigma_{i+1}^y)/2 = (2c_i^\dagger c_i - 1)c_{i+1} \\ \sigma_{i+1}^z &= 2c_{i+1}^\dagger c_{i+1} - 1 \end{aligned} \quad (13)$$

in which $\mathbf{i} + 1$ denotes the nearest neighbor lattice for site \mathbf{i} . This point can be explained as the following. The difficulty for the JW transformation in higher dimension case comes from the absence of a natural ordering of particles. However when one focuses on the nearest neighbored particle, this difficulty does not appear since for a definite direction the nearest neighbor particle is unique (for non-nearest neighbored case one have to consider the effect from the other particles). Then the correlation functions for the ground state are in this case

$$\begin{aligned} p_{00} &= 1, p_{30} = 1 - \frac{2}{L} \sum_{\mathbf{k}} h_{\mathbf{k}\mathbf{i}}^2; p_{03} = 1 - \frac{2}{L} \sum_{\mathbf{k}} h_{\mathbf{k}(\mathbf{i}+1)}^2; \\ p_{11} &= \frac{2}{L} \sum_{\mathbf{k}} (h_{\mathbf{k}\mathbf{i}} - g_{\mathbf{k}\mathbf{i}})(h_{\mathbf{k}(\mathbf{i}+1)} + g_{\mathbf{k}(\mathbf{i}+1)}); \\ p_{22} &= \frac{2}{L} \sum_{\mathbf{k}} (h_{\mathbf{k}\mathbf{i}} + g_{\mathbf{k}\mathbf{i}})(h_{\mathbf{k}(\mathbf{i}+1)} - g_{\mathbf{k}(\mathbf{i}+1)}) \\ p_{33} &= (1 - \frac{2}{L} \sum_{\mathbf{k}} h_{\mathbf{k}\mathbf{i}}^2)(1 - \frac{2}{L} \sum_{\mathbf{k}} h_{\mathbf{k}(\mathbf{i}+1)}^2) \\ &\quad + \frac{4}{L^2} \sum_{\mathbf{k}, \mathbf{k}'} h_{\mathbf{k}\mathbf{i}} h_{\mathbf{k}(\mathbf{i}+1)} g_{\mathbf{k}'\mathbf{i}} g_{\mathbf{k}'(\mathbf{i}+1)} - h_{\mathbf{k}\mathbf{i}} g_{\mathbf{k}\mathbf{i}} h_{\mathbf{k}'(\mathbf{i}+1)} g_{\mathbf{k}'\mathbf{i}} \\ p_{12} &= p_{21} = 0 \end{aligned} \quad (14)$$

2.2 Geometric Phase

Following the method in Refs. [12, 13], one can introduce a globe rotation $R(\phi) = \exp[i\phi \sum_i c_i^\dagger c_i]$ to obtain the ge-

ometric phase(GP). Then we have Hamiltonian with parameter ϕ

$$H(\phi) = \sum_{\mathbf{ij}} c_i^\dagger A_{ij} c_j + \frac{1}{2} (c_i^\dagger B_{ij} c_j^\dagger e^{2i\phi} + \text{h.c.}), \quad (15)$$

and the ground state becomes $|g(\phi)\rangle = R(\phi)|g\rangle$. GP is defined as [10]

$$\begin{aligned} \gamma_g &= -i \int d\phi \langle g(\phi) | \frac{\partial}{\partial \phi} | g(\phi) \rangle \\ &= \frac{\phi}{L} \sum_{\mathbf{i}} \sum_{\mathbf{k}} h_{\mathbf{k}\mathbf{i}}^2 \end{aligned} \quad (16)$$

Regarding to Eq.(15), one only require $\phi = \pi$ for a cycle evolution. Hence one has $\gamma_g = \frac{\pi}{L} \sum_{\mathbf{i}} \sum_{\mathbf{k}} h_{\mathbf{k}\mathbf{i}}^2 = \frac{1}{L} \sum_{\mathbf{i}} \gamma_{gi}$.

2.3 GP vs. Concurrence

At a glance of Eq.(12) and Eq.(16), GP and concurrence both are related directly to correlation functions. Hence it is tempting to find the relation between the two quantities, which would benefit to the understanding of the physical meaning of concurrence.

According to Eqs.(12) and (14), the following inequality can be obtained (see Appendix for details of calculations)

$$\begin{aligned} c_I &\leq \frac{1}{L\pi} (\gamma_{gi} + \gamma_{g(\mathbf{i}+1)}) - \sqrt{(1 + p_{33})^2 - (p_{30} + p_{03})^2} \\ c_{II} &\leq 1 + \frac{1}{L\pi} (\gamma_{gi} - \gamma_{g(\mathbf{i}+1)}) - \frac{1}{2L^2\pi^2} (\gamma_{gi} - \gamma_{g(\mathbf{i}+1)})^2 \end{aligned} \quad (17)$$

For the first inequality, a much tighter bound is difficult to find. While if the average of c_{II} over all site \mathbf{i} is considered, $c_{II} \leq 1 - \frac{1}{2L^3\pi^2} \sum_i (\gamma_{gi} - \gamma_{g(\mathbf{i}+1)})^2$. Fortunately in the following examples c_I is always negative. Although the existence of this defect, in our own points, the relation between GP and concurrence have been displayed genuinely from the inequality above.

3 GP and Concurrence in Higher Dimensional XY model

The previous section presents the general discussion of GP and concurrence in free fermion lattice system Eq.(1). In this section a concrete model would be checked explicitly, of which the Hamiltonian is

$$H = \sum_{\langle \mathbf{i}, \mathbf{j} \rangle} [c_i^\dagger c_j - \gamma (c_i^\dagger c_j^\dagger + \text{h.c.})] - 2\lambda \sum_{\mathbf{i}} c_i^\dagger c_i, \quad (18)$$

in which $\langle \mathbf{i}, \mathbf{j} \rangle$ denotes the nearest-neighbor lattice sites and c_i is fermion operator. This Hamiltonian, first introduced in Ref. [29], depicts the hopping and pairing between nearest-neighbor sites in hypercubic lattice systems, in which λ is the chemical potential and γ is the pairing

potential. Eq.(18) could be considered as a d -dimensional generalization of 1D XY model. However for $d > 1$ case, this model shows different phase features [29].

The Hamiltonian can be diagonalized by introducing the d -dimensional Fourier transformation with periodic boundary condition in momentum space [29]

$$H = \sum_{\mathbf{k}} 2t_{\mathbf{k}} c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} - i\Delta_{\mathbf{k}} (c_{\mathbf{k}}^{\dagger} c_{-\mathbf{k}}^{\dagger} - \text{h.c.}), \quad (19)$$

in which $t_{\mathbf{k}} = \sum_{\alpha=1}^d \cos k_{\alpha} - \lambda$ and $\Delta_{\mathbf{k}} = \gamma \sum_{\alpha=1}^d \sin k_{\alpha}$. With the help of Bogoliubov transformation, one obtains

$$H = \sum_{\mathbf{k}} 2\Lambda_{\mathbf{k}} \eta_{\mathbf{k}}^{\dagger} \eta_{\mathbf{k}} + \text{const.} \quad (20)$$

in which $\Lambda_{\mathbf{k}} = \sqrt{t_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}$. Based on the degeneracy of the eigenenergy $\Lambda_{\mathbf{k}} = 0$, the phase diagram can be determined clearly [29]; When $d = 2$, the phases diagram should be identified as two different situations; for $\gamma = 0$, the degeneracy of the ground state occurs when $\lambda \in [0, 2]$, whereas the gap above the ground state is non-vanishing for $\lambda > 2$. However for $\gamma \neq 0$ three different phases can be identified as $\lambda = 0$, $\lambda \in (0, 2]$ and $\lambda > 2$. The first two phases correspond to case that the energy gap above the ground state vanishes, whereas not for $\lambda > 2$. One should note that $\lambda = 0$ means a well-defined Fermi surface with $k_x = k_y \pm \pi$, whose symmetry is lowered by the presence of λ term. For $d = 3$ two phases can be identified as $\lambda \in [0, 3]$ with the vanishing energy gap above the ground state and $\lambda > 3$ with a non-vanishing energy gap above ground state. In a word the critical points can be identified as $\lambda_c = d(d = 1, 2, 3)$ for any anisotropy of γ , and $\lambda = 0$ for $d = 2$ with $\gamma \neq 0$. One should note that since the γ^2 dependence of $\Lambda_{\mathbf{k}}$, the sign of γ does not matter. Hence the plots below are only for positive γ .

The correlation functions between nearest-neighbor lattice sites would play a dominant role in the transition between different phases because of the nearest-neighbor interaction, similar to the case in XY model [3]. Then it is expected that the pairwise entanglement is significant in this model. In the following, concurrence for the nearest-neighbor sites of ground state is calculated for $d = 2, 3$ respectively. The geometric phase of ground state is also calculated by imposing a globe rotation $R(\phi)$. our calculation shows that both quantities show interesting singularity closed to the boundary of different phases.

3.1 Concurrence

For $d > 1$ case, the nearest-neighbor lattice sites appear in different directions. In order to eliminate the dependence of orientations, the calculation of correlation functions Eqs.(14) is implemented by averaging in all directions. With the transformation Eq.(13), one can determine

under the thermodynamic limit

$$\begin{aligned} p_{11} &= \frac{1}{d(2\pi)^d} \int_{-\pi}^{\pi} \prod_{\alpha} dk_{\alpha} (\Delta_{\mathbf{k}} \sum_{\alpha=1}^d \sin k_{\alpha} - t_{\mathbf{k}} \sum_{\alpha=1}^d \cos k_{\alpha}) / \Lambda_{\mathbf{k}} \\ p_{22} &= -\frac{1}{d(2\pi)^d} \int_{-\pi}^{\pi} \prod_{\alpha} dk_{\alpha} (\Delta_{\mathbf{k}} \sum_{\alpha=1}^d \sin k_{\alpha} + t_{\mathbf{k}} \sum_{\alpha=1}^d \cos k_{\alpha}) / \Lambda_{\mathbf{k}} \\ p_{12} &= p_{21} = 0 \\ p_{03} &= p_{30} = p_3 = \frac{1}{(2\pi)^d} \int_{-\pi}^{\pi} \prod_{\alpha} dk_{\alpha} \frac{t_{\mathbf{k}}}{\Lambda_{\mathbf{k}}} \\ p_{33} &= p_3^2 - \left(\frac{p_{11} + p_{22}}{2}\right)^2 + \left(\frac{p_{11} - p_{22}}{2}\right)^2 \end{aligned} \quad (21)$$

$d = 2$ Our calculation shows that c_{II} is negative. So in Fig. 1, only c_{II} and its derivative with λ are numerically illustrated. In order to avoid the ambiguity because of the cutoff in the definition of concurrence, the derivative of c_{II} with λ is depicted in all region whether c_{II} positive or not [7]. Obviously the singularity for $\partial c_{II} / \partial \lambda$ can be found at the point $\lambda = 0, 2$ respectively, which are consistent with our knowledge about phase transitions.

$d = 3$ Similar to the case of $d = 2$, our calculation shows $c_I < 0$. Only c_{II} and its derivative with λ are numerically displayed in Fig.2. Different from the case of $d = 2$, no singularity of the first derivative of c_{II} with λ is found at $\lambda = 3$. While a cusp appears at $\lambda = 1$. A further calculation demonstrates that the second derivative of c_{II} is divergent genuinely at exact $\lambda = 3$, as shown in Figs.2(c). which means the phase transition at this points. Furthermore our numerical calculations show that $\partial^2 c_{II} / \partial \lambda^2$ is finite at $\lambda = 1$, as shown in Figs.2(b). Hence one cannot attribute this feature to the phase transition. The similar feature has been found in the previous studies [3, 7, 30]. However the underlying physical reason is unclear in general. But this special feature is not unique for concurrence; van Hove singularity in solid state physics displays the similar feature, which is because of the vanishing of the moment-gradient of the energy. Although we cannot established the direct relation between these two issues because of the bad definition of the moment-gradient of the energy when degeneracy happening, we affirm that this feature is not an accident and the underlying physical reason is still to be found.

In a word the discussion above first demonstrates the exact connection between concurrence and quantum phase transitions in high-dimensional many body systems. However a question is still open; what the physical interpretation of concurrence is in many-body systems. In this study, we includes the negative part of c_{II} to identify the phase diagram in free-fermion systems. In general, it is believed that the negative c_{II} means no entanglement between two particles and then include no any useful information about state. But from the discussion one can note that the omission of the negative part of c_{II} would lead to incorrect results. Moreover, for $\gamma = 0$, our calculations show that c_I, c_{II} always are zero, and so one cannot obtain any the phase transition information from pair wise entanglement

in this case. Further discussions will be presented in the final part of this paper.

3.2 Geometric Phase

Geometric phase manifests the structure of Hilbert in the system and has intimate relation to the degeneracy. GP, defined in Eq. (16) by imposing a globe rotation $R(\phi)$ on ground state $|g\rangle$ is calculated in this section. After some algebra, one obtains

$$\gamma_g = \frac{\pi}{2(2\pi)^d} \int_{-\pi}^{\pi} \prod_{\alpha=1}^d dk_{\alpha} \left(1 - \frac{t_k}{\Lambda_k}\right). \quad (22)$$

$d = 2$ In Fig.3, γ_g and its derivative with λ are displayed explicitly. Obviously one notes that $\partial\gamma_g/\partial\lambda$ shows the singularity closed to $\lambda = 0, 2$, which are exactly the phase transition points of Hamiltonian Eq.(18). An interesting observation is that closed to these points, both GP and concurrence c_{II} show the similar behaviors.

$d = 3$ GP and its derivative are plotted explicitly in Fig.(4). One should note that there is a platform below $\lambda = 1$ for $\partial\gamma_g/\partial\lambda$, as shown in Fig.4(a), but a further calculation shows that $\partial^2\gamma_g/\partial\lambda^2$ is continued (Fig.4(b)) and $\partial\gamma_g/\partial\lambda$ has no divergency at this point. This phenomena is very similar to the case of concurrence (see Fig.2(b, c)). As expected, $\partial^2\gamma_g/\partial\lambda^2$ is divergent at exact $\lambda = 3$, which means a phase transition happens at this point. Together with respect of the case of $d = 2$, it makes us a suspect that GP and concurrence in our model have the same physical origination.

Furthermore for $\gamma = 0$, GP fails to mark the phase transition too. This is similar to the case of concurrence, but has different physical reason. The further discussion is presented in the next section.

4 Discussion and Conclusions

The pairwise entanglement and geometric phase for ground state in d -dimensional ($d = 2, 3$) free-fermion lattice systems are discussed in this paper. By imposing the transformation Eq.(13), the reduce two-body density matrix for the nearest neighbor particles can be determined exactly for any dimension, and the concurrence is also calculated explicitly. Furthermore geometric phase for ground state, obtained by introducing a globe rotation $R(\phi)$, has also been calculated. Given the known results for XY model [3, 12, 13], our calculations show again that both GP and concurrence display intimate connection with the phase transitions. Moreover an inequality relation between concurrence and geometric phase is also presented in Eq. (17). The similar scaling behaviors at the transition point $\lambda = 3$ has also been shown in Figs. 5. These facts strongly mean the intimate connection between the two items. This point can be understand by noting that both of them are connected to the correlation functions, as shown in Eqs. (12) and (16).

An interesting point in our study is that in order to obtain all information of phase diagram in model Eq.(18), the negative part of c_{II} has to be included to avoiding the confusion because of the mathematical cutoff in the definition of concurrence [7]. In general, it is well accepted that the negative part of c_{II} gives no any information of quantum pairwise entanglement, and then is considered to be meaningless. However, in our calculation, the negative part of c_{II} appears as an indispensable consideration to obtain the correct phase information. This point means that the pairwise entanglement does not provide the all information about the system since the two-body reduced density operator throw away much information.

As for the geometric phase, defined in Eq. (16), it is obvious that γ_g can tell us the happening of phase transition at the point, where γ_g display some kinds of singularity. However it cannot distinguished the degenerate region from the nondegenerate, as shown in Figs. 3 and 4. Recently GP imposing by the twist operator in many-body systems is introduced as an order parameter to distinguish the phases [17, 18]. For the free-fermion lattice system, this GP have also calculated and shows the intimate connection with the vanishing of energy gap above the ground state. However the boundary between the two different phases becomes obscure with the increment of dimensionality in that discussion [17], and moreover it cannot distinguish the phase transition not come from the degeneracy of the ground-state energy. While the geometric phase imposing by the globe rotation $R(\phi)$ clearly demonstrate the existence of this kind of phase transition, as shown in Fig.3, whether originated from the degeneracy or not. In fact this point can be understood by noting the intimate relation between γ_g and correlation functions. It maybe hint that one has to find different methods for different many-body systems to identify the phase diagram.

Although the intimate relationship of concurrence and GP with phase transitions in the model Eq.(18), a exceptional happens when $\gamma = 0$, in which c_I, c_{II} are zero and GP is a constant independent of λ . From Eq.(18), $\gamma = 0$ means the hopping of particles is dominant, and the position of particle becomes meaningless. Since the calculation of concurrence depend on the relative position of lattice site, the pairwise entanglement is disappearing. However one could introduce the spatial entanglement to detect the phase transition in this case [31]. For GP, $\gamma = 0$ means the emergency of new symmetry. One can find $[\sum_i c_i^\dagger c_i, H] = 0$ in this case, which leads to the failure of $R(\phi)$ for construction of nontrivial GP.

Finally we try to transfer two viewpoints in this paper. One is that concurrence and geometric phase can be used to mark the phase transition in many-body systems since both of them are intimately connected to the correlation functions. The other is that concurrence and the geometric phase are connected directly by the inequality Eq. (17). Then it is interesting to extend this relation to multipartite entanglement in the future works, which would be helpful to establish the physical understanding of entanglement.

The author (Cui) would appreciate the help from Dr. Kai Niu (DLUT) and Dr. Chengwu Zhang (NJU) in the numerical calculations and permission of the usage of their powerful computers. We also thank greatly the enlightening discussion with Dr. Chong Li (DLUT). Especially we thank the first referee for his/her important hint for the van Hove singularity. This work is supported by the Special Foundation of Theoretical Physics of NSF in China, Grant No. 10747159.

APPENDIX

For the first inequality, one should note

$$\begin{aligned} & |p_{11} + p_{22}| \\ &= \frac{4}{L} \left| \sum_{\mathbf{k}} h_{\mathbf{k}i} h_{\mathbf{k}(i+1)} \right| \leq \frac{4}{L} \sum_{\mathbf{k}} |h_{\mathbf{k}i} h_{\mathbf{k}(i+1)}| \\ &\leq \frac{2}{L} \sum_{\mathbf{k}} (h_{\mathbf{k}i}^2 + h_{\mathbf{k}(i+1)}^2) = \frac{2}{L\pi} (\gamma_{gi} + \gamma_{g(i+1)}). \end{aligned} \quad (23)$$

From inequality $\sqrt{x^2 - y^2} \geq |x| - |y|$ ($|x| > |y|$), one reduces

$$\sqrt{(1 + p_{33})^2 - (p_{30} + p_{03})^2} \geq |1 + p_{33}| - |p_{30} + p_{03}|. \quad (24)$$

Then one obtains

$$c_I \leq \frac{1}{L\pi} (\gamma_{gi} + \gamma_{g(i+1)}) + \frac{1}{2} (|p_{30} + p_{03}| - |1 + p_{33}|). \quad (25)$$

However a much tighter bound is difficult to decide because of the complexity of p_{33} .

For the second inequality, it can be obtained easily by observing

$$p_{33} \leq 1 - \frac{1}{L^2\pi^2} (\gamma_{gi}^2 - \gamma_{g(i+1)}^2), \quad (26)$$

in which we have used the relation $2ab \leq a^2 + b^2$. Then $1 - p_{33}$ is non-negative and

$$\begin{aligned} c_{II} &= \frac{2}{L} \sum_{\mathbf{k}} |h_{\mathbf{k}i} g_{\mathbf{k}(i+1)}| + \frac{p_{33} - 1}{2} \\ &\leq \frac{1}{L} \sum_{\mathbf{k}} (h_{\mathbf{k}i}^2 + g_{\mathbf{k}(i+1)}^2) - \frac{1}{2L^2\pi^2} (\gamma_{gi} - \gamma_{g(i+1)})^2 \\ &\leq 1 + \frac{1}{L\pi} (\gamma_{gi} - \gamma_{g(i+1)}) - \frac{1}{2L^2\pi^2} (\gamma_{gi} - \gamma_{g(i+1)})^2 \end{aligned} \quad (27)$$

in which $1/L \sum_{\mathbf{k}} g_{\mathbf{k}i}^2 = 1 - 1/L \sum_{\mathbf{k}} h_{\mathbf{k}i}^2$ is used.

References

1. L. Amico, R. Fazio, A. Osterloh, V. Vedral, Rev. Mod. Phys. **80**, 517 (2008) and available at arXiv: quant-ph/0703044(2007).
2. J. Preskill, J. Mot. Opt. **47**, (2000)127.
3. A. Osterloh, L. Amico, G. Falci, R. Fazio, Nature, **416**, 6(2002)08; T. J. Osborne and M. A. Nielsen, Phys. Rev. A **66**, (2002)032110.

4. X. X. Yi, H. T. Cui and L. C. Wang, Phys. Rev. A **74**, (2006)054102.
5. H.T. Quan, Z. Song, X.F. Liu, P. Zanardi, C.P. Sun, Phys. Rev. Lett. **96**, (2006)140604.
6. P. Zanardi and N. Paunković, Phys. Rev. E **74**, 031123 (2006); P. Zanardi, P. Giorda, M. Cozzini, Phys. Rev. Lett. **99**, (2007)100603; Shi-Jian Gu, e-print available at arXiv: 0811.3127.
7. M. F. Yang, Phys. Rev. A **71**, (2005)030302.
8. V. Vedral, J. Mod. Opt. **54**, 2185(2007).
9. M. R. Dowling, A. C. Doherty, and S. D. Bartlett, Phys. Rev. A **70**, (2004)062113; Wieśniak, V. Vedral, and časlav Brukner, New. J. Phys. **7**, 2005258.
10. M. V. Berry, Proc. R. Soc. London A **392**, (1984)45.
11. A. Shapere and F. Wilczek, *Geometric Phase in Physics* (World Scientific, 1989); A. Bohm, A. Mostafazadeh, H. Koizumi, Q. Niu, J. Zwanziger, *The Geometric Phase in Quantum System*(Springer, 2003).
12. Angelo C. M. Carollo, J. K. Pachos, Phys. Rev. Lett. **95**, (2005)157203; J. K. Pachos, Angelo C. M. Carollo, Phil. Trans. R. Soc. A **364**, 3463(2006).
13. S. L. Zhu, Phys. Rev. Lett. **96**, (2006)077206.
14. A. Hama, arXiv: quant-ph/0602091.
15. H.T. Cui, K. Li, and X.X. Yi, Phys. Lett. A **360**, (2006)243.
16. F. Plastina, G. Liberti, A.Carollo, Europhys.Lett. **76**, (2006)182.
17. H.T. Cui, J. Yi, Phys. Rev. A **78**, (2008)022101.
18. T. Hirano, H. Katsura, and Y. Hatsugai, Phys. Rev. B **77**, (2008)094431; Phys. Rev. B **78**, (2008)054431.
19. S.L. Zhu, Int. J. Mod. Phys. B **22**, (2008)561.
20. Subir Sachdev, *Quantum Phase Transition*(Cambridge University Press, Cambridge, 1999).
21. S. Q. Shen, Phys. Rev. B **70**, (2004)081311; M. C. Chang, Phys. Rev. B **71**, (2005)085315; T.W. Chen, C.M. Huang, G. Y. Guo, Phys. Rev. B, **73**, (2006)235309; D. N. Sheng, Z. Y. Weng, L. Sheng, F. D. M. Haldane, Phys. Rev. Lett.**97**, (2006)036808; B Zhou, C.X. Liu, S.Q. Shen, Europhys. Lett. **79**, (2007)47010.
22. T. Senthil, Proceedings of conference on ‘Recent Progress in Many-Body Theories’, Santa Fe, New Mexico (USA, 2004).
23. S. Ryu, Y. Hstsugai, Phys. Rev. B **73**, (2006)245115.
24. S. Bose, Phys. Rev. Lett. **91**, (2003)207901; Z. Song and C.P. Sun, Low Temperature Physics, **31**, (2005)8.
25. E. Lieb, T. Schultz and D. Mattis, Ann. Phys. **16**, (1961)407.
26. W. K. Wootters, Phys. Rev. Lett. **80**, (1998)2245.
27. P. Jordan and E. Wigner, Z. Physik **47**, (1928)631.
28. E. Fradkin, Phys. Rev. Lett. **63**, 322(1989); Y.R. Wang, Phys. Rev. B, **43**, (1991)3786; L. Huerta and J. Zanelli, Phys. Rev. Lett. **71**, (1993)3622; Shaofeng Wang, Phys. Rev. E, **51**, (1995)1004; C.D. Batista and G. Ortiz, Phys. Rev. Lett, **86**, (2001)1082; Adv. in Phys. **53**, (2004)1.
29. W.F. Li, L.T. Ding, R. Yu, T. Roscide, S. Haas, Phys. Rev. B **74**, (2006)073103.
30. S.J. Gu, G.S. Tian, H.Q. Lin, Phys. Rev. A **71**, (2004)052332; Chin. Phys. Lett. **24**, (2007)2737.
31. P. Zanardi, Phys. Rev. A **65**, 042101(2002).

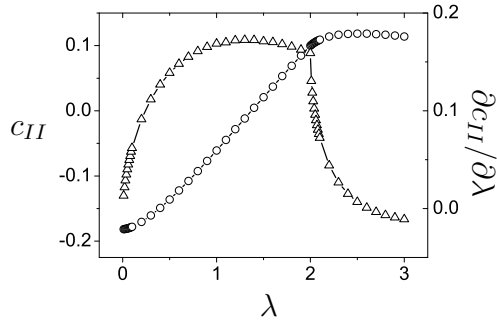


Fig. 1. c_{II} (\circ) and its derivative with λ (\triangle) vs. λ when $d = 2$. We have chosen $\gamma = 1$ for this plot.

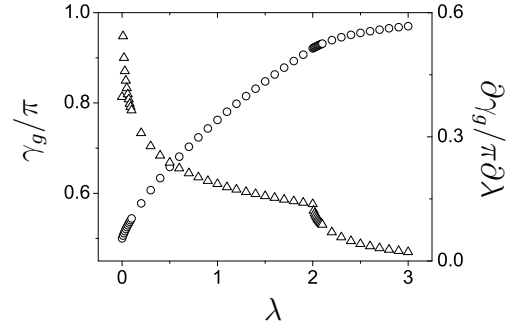


Fig. 3. γ_g (\circ) and its derivative with λ (\triangle) vs. λ when $d = 2$. We have chosen $\gamma = 1$ for this plot.

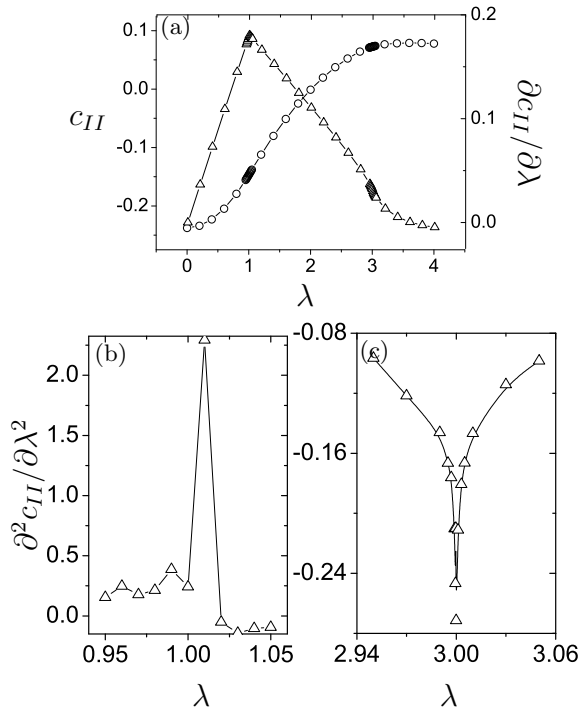


Fig. 2. c_{II} (\circ) and its derivative with λ (\triangle) (a) vs. λ when $d = 3$. We have chosen $\gamma = 1$ for this plot. The second derivative of c_{II} with λ are also displayed in this plot and focus the points closed to $\lambda = 1$ (b) and $\lambda = 3$ (c).

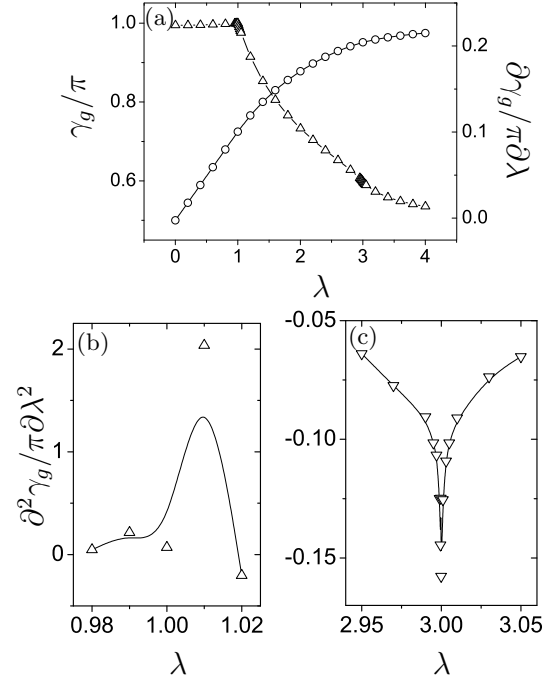


Fig. 4. γ_g (\circ) and its derivative with λ (\triangle) (a) vs. λ when $d = 3$. We have chosen $\gamma = 1$ for this plot. The second derivative of γ_g with λ are also displayed in this plot and focus the points closed to $\lambda = 1$ (b) and $\lambda = 3$ (c).

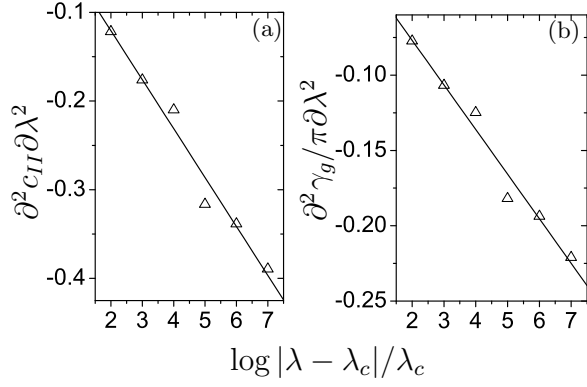


Fig. 5. The scaling of GP and concurrence for 3D case closed to the critical point $\lambda_c = 3$. We have chosen $\gamma = 1$ for this plot.